Assessing the Effectiveness of Acceleration Methods for Deterministic Neutron Transport Solvers

Building a new tool for developers.

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ANS Summer Meeting: Acceleration Methods

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A majority of our limited time and effort (and funding) should be dedicated to designing new and better acceleration methods, **not implementing and analyzing results**.

Outline

1. Why acceleration methods?
2. Analysis and implementation challenges
3. Design paradigm
4. Status and future work
5. Backup Slides

Steady-state Boltzman Transport Equation

Our problem of interest is the time-independent transport equation on a domain of interest $\mathbf{r} \in V$ [3],

$$\left[\hat{\Omega} \cdot \nabla + \Sigma_t(\mathbf{r}, E)\right] \psi(\mathbf{r}, E, \hat{\Omega}) \\ = \int_0^\infty dE' \int_{4\pi} d\hat{\Omega}' \Sigma_s(\mathbf{r}, E' \to E, \hat{\Omega}' \to \hat{\Omega}) \psi(\mathbf{r}, E', \hat{\Omega}') \\ + Q(\mathbf{r}, E, \hat{\Omega}) \ ,$$

with a given boundary condition,

$$\psi(\mathbf{r}, E, \hat{\Omega}) = \Gamma(\mathbf{r}, E, \hat{\Omega}), \quad \mathbf{r} \in \partial V, \quad \hat{\Omega} \cdot \hat{n} < 0$$

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Gauss-Seidel source iteration $\mathbf{\Psi}_{(k+1)} = \mathbf{L}^{-1}\mathbf{M}\left[\mathbf{S}\mathbf{\Phi}_{(k)} + \frac{1}{k}\mathbf{F}\mathbf{\Phi}_{(0)}\right]$

Power iteration $\mathbf{\Psi}_{(k+1)} = \mathbf{L}^{-1}\mathbf{M}\left[\mathbf{S}\mathbf{\Phi}_{(0)} + \frac{1}{k}\mathbf{F}\mathbf{\Phi}_{(k)}\right]$

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Power iteration can convergence arbitrarily slow as the dominance ratio k_1/k_0 approaches unity.

Motivates the development of **acceleration methods** to address these issues.

- Source Iteration: Diffusion two-grid method (TG).
- Power Iteration: Nonlinear diffusion acceleration (NDA).

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with total computational work

$$W = \sum_{\ell=1}^{N} w_{(\ell)} \ .$$

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Note

The same amount of error needs to be removed for the problem to converge, regardless of the method used to remove it.

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What do we need?

A coding framework designed with the developer end-user in mind, that is portable and reproducible.

Defining work

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In general, we use inversions of the transport matrix – explicitly or implicitly (*sweeps*) – as a unit of work.

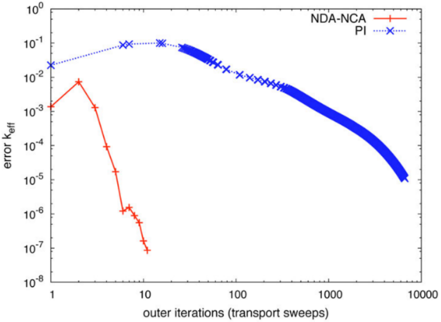

Figure 1: NDA convergence vs standard power iteration [7]

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This becomes complicated as our acceleration methods become more complex, and take on more work.

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What do we need?

Additional, good data that enables us to assess the effectiveness of our method.

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- Combined or complex schemes may invalidate assumptions.
- Implementation and reproducibility can be difficult.

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1. relieves some of the burden of implementing a novel acceleration method,
2. provides a controlled environment for measuring the effectiveness of the novel method, and,
3. provides tools for verifying the basis for effectiveness.

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Goal 1

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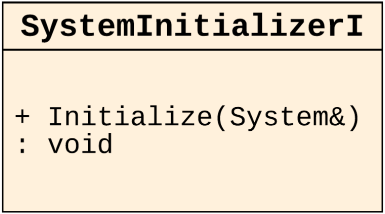

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- Comprehensive testing coverage.

Controlled testing environment

Goal 2

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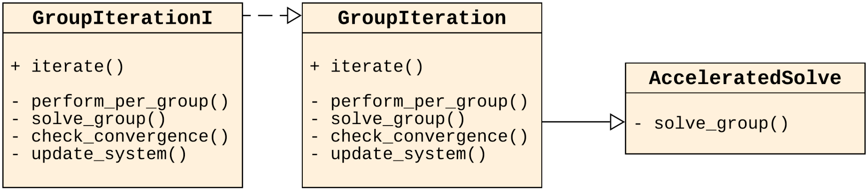

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- Enables a true comparison of the accelerated solve to a control solve.
- Makes the modifications *portable*.
- Enables us to compare the implementation of the method to dis-aggregate the computer science from the method itself.

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BART will include the ability to *instrument* a solve to gather enough data to draw useful conclusions about the effectiveness of acceleration schemes.

- Storage of solve parameters (eigenvalues, fluxes).
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Adding new instrumentation must be easy!

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- Uses the Google Protocol Buffers file format for cross-sections.

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- Instrumentation in development: *in-situ* stepwise Fourier Analysis.

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- We are developing a new code aimed at helping developers of new methods.
- We hope that the code will ease the burden of coding up new methods, and help provide good, useful data for understanding if and why the methods are worthwhile to implement in production level codes.

Thank you

References

[1] B. T. Adams and Jim E. Morel.
A Two-Grid Acceleration Scheme for the Multigroup Sn Equations with Neutron Upscattering.
Nuclear Science and Engineering, 115(May):253–264, 1993.

[2] Satish Balay, William D. Gropp, Lois Curfman McInnes, and Barry F. Smith.
Efficient management of parallelism in object oriented numerical software libraries.
In E. Arge, A. M. Bruaset, and H. P. Langtangen, editors, *Modern Software Tools in Scientific Computing*, pages 163–202. Birkhäuser Press, 1997.

[3] E. E. Lewis and W.F. Miller, Jr.
Computational Methods of Neutron Transport.
American Nuclear Society, 1993.

[4] G. Alzetta et al.
The `deal.II` library, version 9.0.
Journal of Numerical Mathematics, 26(4):173–183, 2018.

[5] Thomas M. Evans, Kevin T. Clarno, and Jim E. Morel.
A Transport Acceleration Scheme for Multigroup Discrete Ordinates with Upscattering.
Nuclear Science and Engineering, 165:292–304, 2010.

[6] Google.
Googletest – Google Testing and Mocking Framework.
`https://github.com/google/googletest`.
Accessed: 2017 December 20.

[7] H. Park, D. A. Knoll, and C. K. Newman.
Nonlinear Acceleration of Transport Criticality Problems.
Nuclear Science and Engineering, 172(1):52–65, 2012.

[8] et al. Satish Balay.
PETSc users manual.
Technical Report ANL-95/11 - Revision 3.12, Argonne National Laboratory, 2019.

[9] et al. Satish Balay.
PETSc Web page.
`https://www.mcs.anl.gov/petsc`, 2019.

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